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TRANSPORT THEORY FOR HEAVY ION BEAMS NEAR A TARGET SURFACE.(U)

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The method of Manning and Padgett (MP) for studying the transport of heavy ion beams in amorphous solids is modified to allow for inelastic (electronic) slowing of the ion beam as well as the losses from elastic scattering. The MP method consists of writing the distribution function that satisfies the Boltzmann transport equation in a form that reflects the physical processes that the beam ions undergo as they enter the target. In our version of this method, the beam distribution function consists of several terms with the

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20. Abstract (Continued)

following characteristics: n terms that represent beam ions that have undergone exactly zero, one, two, ... , n—1 elastic collisions, and a final term that represents beam ions that have undergone n or more elastic collisions. In the present work the formal solutions of the Boltzmann equation are given for these various terms. The explicit forms for the first two terms are presented and the results of sample calculations are reported.

CONTENTS

TRANSPORT THEORY FOR HEAVY ION BEAMS NEAR A TARGET SURFACE

I. INTRODUCTION

When treated from the point of view of transport theory, the bombardment of a target by a beam of energetic particles involves highly singular functions, where by singular functions we mean either Dirac delta functions or functions that are sharply peaked in one or more of the independent variables. At the penetrating surface the distribution function for the penetrating particles has Dirac delta functions in energy and angle corresponding to the monoenergetic and paraxial nature of the bombarding beam. In this work we undertake a systematic treatment of these singularities.[1] We show that, if one is interested in a numerical calculation of the distribution function, numerical approximations to the singular functions can be avoided by systematically extracting them and treating them exactly. We also show how our approach naturally leads to an iterative (successive scattering) treatment of the distribution function near the penetrating surface that could be the basis of a self-contained transport theory of near-surface phenomena in ion bombardment.

The transport theory for penetration of an amorphous target is formulated in the next section. Our approach, which is based on the Boltzmann equation, is familiar to workers in neutron transport theory.[2-4] Specifically, our approach parallels and was suggested by that of Manning and Padgett (MP).[5] In contrast, much of the recent work on ion bombardment[6-9] utilizes a transport equation of the type used by Lindhard, Scharff, and Schiott (LSS).[10] Our treatment of the inelastic collisions is that of LSS.

In Section III we show that the distribution function can be split into a hierarchy of terms of decreasing singularity: a ψ_0 term, which represents the beam as it first enters the target, wherein it loses energy

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to inelastic processes but retains its unidirectional character; terms ψ_1, ψ_2, ..., ψ_{n-1}, which represent beam ions that have undergone one, two, ..., n-1 elastic collisions; and a Φ_n term, which represents beam ions which have undergone n or more elastic collisions. The explicit solutions for the first two terms are given in Secs. IV and V. The formal solutions for the remaining ψ_s terms, s = 2,3,...,n-1, and the equation that must be solved for Φ_n are discussed in Sec. VI. The following section presents the results of some sample numerical calculations for ψ_0 and ψ_1, using the Lindhard cross sections.[10] Section VIII contains our concluding remarks and a discussion of a number of possible extensions of this work.

The conceptual form of the solution of the Boltzmann equation that we use (Sec. III) is the same as that of Manning and Padgett. The solution for the most singular term, the ψ_0 term, is also the same as that of MP, although the derivation is different. Our version of the ψ_1 term differs somewhat from that of MP; it provides a complete description of particles that have undergone one elastic collision while suffering the effects of the continuous inelastic losses. The iteration method of Sec. VI for solving for successive ψ_s terms is similar to that discussed by MP, but the present effort provides formal expressions for the result of each iteration.

The continuous energy loss model for inelastic collisions used by LSS[10] is further discussed in Appendix A. Our presentation is based on the work of Symon,[11] and follows that of Ref. 5. Appendix B contains a brief description of the LSS cross section,[10] using our notation.

II. BOLTZMANN EQUATION FOR BEAM PENETRATION

For convenience, we repeat here the formulation of the Boltzmann equation for beam penetration as found in MP.[5] Consider a beam of heavy ions of charge Z_1, mass m_1, and energy E_B penetrating an amorphous target made up of atoms of charge Z_2 and mass m_2, with number density N. Following the notation of Case and Zweifel,[2] we take the single particle distribution function to be $\chi(\mathbf{r},\mathbf{v},t)$ where

$\chi(\underline{r},\underline{v},t)$ = the number of particles in d^3r about $\underline{r}$ and d^3v about $\underline{v}$ at time t. (1)

The function $\sigma(\underline{v}'\rightarrow\underline{v})$ is defined as follows:

$N\,\sigma(\underline{v}'\rightarrow\underline{v})\,v'\,\chi(\underline{r},\underline{v}',t)\,d^3r\,d^3v\,dt\,d^3v'$ = the probable number of beam particles of velocity in d^3v' about $\underline{v}'$, located in d^3r about $\underline{r}$, which undergo a collision in time dt about t such that their final velocities lie in d^3v about $\underline{v}$. (2)

Since $\underline{v}\,\chi(\underline{r},\underline{v},t)$ is the flux of particles with velocity $\underline{v}$, we see that $\sigma(\underline{v}'\rightarrow\underline{v})$ is a collision cross section. The total cross section is given by

$$\sigma_s(v') = \int d^3v \quad \sigma(\underline{v}'\rightarrow\underline{v}) \quad . \tag{3}$$

(Note that Case and Zweifel use the various σ quantities to represent macroscopic cross sections, which include the factor N.) By applying the principle of the conservation of particles to the χ function over a time interval dt as $\underline{r}$ is changed to $\underline{r}+d\underline{r}$ and $\underline{v}$ changes to $\underline{v}+d\underline{v}$, one finds[2,5] the Boltzmann transport equation for beam penetration to be

$$\frac{\partial}{\partial t}\chi(\underline{r},\underline{v},t) + \underline{v}\cdot\underline{\nabla}\chi + vN\sigma_s(v)\,\chi = \mathcal{S}(\underline{r},\underline{v},t)$$
$$+ N\int d^3v' \quad \sigma(\underline{v}'\rightarrow\underline{v}) \quad v' \quad \chi(\underline{r},\underline{v}',t) \tag{4}$$

where $\mathcal{S}$ represents the source term for the ion flux.

Throughout the remainder of this paper we will make the simplifying assumptions of rotational invariance, translational invariance, plane symmetry, and time independence. We presume that the beam direction is parallel to the x-axis and that the beam enters the target perpendicular to its face. We let x measure the distance of penetration from the surface and let

$$\mu = \hat{v}\cdot\hat{e}_x \tag{5}$$

represent the cosine of the angle between the beam direction in the target and the initial beam direction. With the above assumptions, the cross sections depend only on E, E', and $\hat{v}\cdot\hat{v}'$. We define a new function $\chi(E,x,\mu)$ that is related to $\chi(\underline{r},\underline{v},t)$ by

$$\chi(E,x,\mu)\,dE\,dx\,d\mu = v^2\,\chi(\underline{r},\underline{v},t)\,dv\,dx\,d\mu \tag{6}$$

and that satisfies the transport equation

$$\mu\frac{\partial}{\partial x}\chi(E,x,\mu) + N\sigma_T(E)\,\chi = \mathcal{S}(E,x,\mu)/v + N\int d^3v'\;\sigma(E,E',\hat{v}\cdot\hat{v}')\;\chi(E',x,\mu') . \tag{7}$$

Because of the assumed time independence, it is simpler to work with the vector flux, rather than the number density $\chi(E,x,\mu)$. In the case of plane symmetry, the vector flux is given by

$$\Psi(E,x,\mu) = \mu\,v\,\chi(E,x,\mu) \tag{8}$$

and it satisfies the Boltzmann equation

$$\mu\frac{\partial}{\partial x}\Psi(E,x,\mu) + N\sigma_T(E)\,\Psi = \mu\,\mathcal{S}(E,x,\mu) + N\mu v\int d^3v'\;(\mu' v')^{-1}\;\sigma(E,E',\hat{v}\cdot\hat{v}')\;\Psi(E',x,\mu') . \tag{9}$$

We now make the widely used assumption[10] that, insofar as the statistics of the transport equation are concerned, the atomic collisions can be modeled as two separate types, inelastic and elastic, and that these two types of collisions occur independently and without interference. Inelastic collisions are thought of as leaving the electrons in the target atom in an excited state, but with the center-of-mass motion of the target atom unperturbed. Elastic collisions are thought of as transferring momentum to the target atom as a whole, while leaving unchanged its electronic state.

Corresponding to this assumption, we can split the cross section into two parts. For the inelastic losses we use the continuous energy loss model,[11] for which the energy loss results from infinitely many collisions, each of which transfers an infinitesimal energy. The direction

of motion of the particles is unaltered by the inelastic losses. The inelastic cross section, which satisfies the relation

$$S(E') = N\int d^3v \; (E'-E) \; \sigma_{in}(E',E,\hat{v}\cdot\hat{v}') \, , \tag{10}$$

is discussed in Appendix A. The function $S(E')$ is called the electronic or inelastic stopping power; it represents the rate of energy loss to inelastic processes. The modifications that this form of continuous loss mechanism generates in the Boltzmann equation appear in Appendix A.

In the case of elastic collisions, wherein the beam ion velocity goes from $\underline{v}'$ to $\underline{v}$, conservation of energy and momentum yield

$$g(E',E) = \tfrac{1}{2}\left[(M+1)(E'/E)^{\frac{1}{2}} - (M-1)(E/E')^{\frac{1}{2}} \right] \tag{11}$$

as the cosine of the scattering angle in the laboratory system, with

$$M = m_2/m_1 \, . \tag{12}$$

The maximum energy transfer in an elastic collision of particles of mass m_1 and m_2 is given by

$$T_{max} = \gamma E' = 4 m_1 m_2 \; (m_1+m_2)^{-2} \quad E' \, , \tag{13}$$

where E' is the energy of the impinging particle. Consequently, the minimum energy for the outgoing particle is

$$E_{min} = E'/\beta = E' \; (m_1-m_2)^2 / (m_1+m_2)^2 \, . \tag{14}$$

We now write the elastic portion of the cross section in the form

$$\sigma_{el}\,(E',E,\hat{v}\cdot\hat{v}') = (2\pi)^{-1} \; \delta(\hat{v}\cdot\hat{v}' - g(E',E)) \; F(E',E) \, . \tag{15}$$

The quantity $F(E',E)$ contains the unit step function $U(\beta E - E')$ due to the kinematical considerations. For convenience, we also define

(16)

The total elastic cross section is now written

$$\sigma_T(E') = \int_{E'/\beta}^{E'} dE \quad \mathcal{F}(E',E) . \tag{17}$$

In the light of the discussion of the last two paragraphs, we obtain the Boltzmann equation in the form

$$\begin{aligned} &\mu \frac{\partial}{\partial x} \Psi(E,x,\mu) + N\sigma_T(E)\Psi - \frac{\partial}{\partial E}\left(S(E)\Psi\right) \\ &= \mu\, \mathcal{S}(E,x,\mu) + \frac{N}{2\pi}\int_E^{\beta E} dE' \quad \mathcal{F}(E',E) \int d\hat{v}' \, \mu'^{-1} \\ &\cdot \delta(\hat{v}\cdot\hat{v}' - g(E',E)) \quad \Psi(E',x,\mu') . \end{aligned} \tag{18}$$

III. FORM OF THE SOLUTION

We assume that the incident beam is perfectly collimated and monochromatic. In particular, we take the source term in Eq. (18) to be

$$\mu\, \mathcal{S}(E,x,\mu) = \mathcal{S}_0 \quad \delta(\mu-1) \ \delta(E-E_0) \ \delta(x) \tag{19}$$

where δ is the Dirac delta function. The source has units of number of particles per unit area per unit time. Since we are examing a time independent problem, all of our results will be proportional to $\mathcal{S}_0$; henceforth we will assume unit incoming flux, i.e., $\mathcal{S}_0 = 1$.

This section outlines the form of the solution $\Psi(E,x,\mu)$ that we choose. The crucial element of this analysis is that we give special attention to the behavior of $\Psi(E,x,\mu)$ near the x=o plane, so that the singular portions of Ψ can be dealt with separately and specifically. Then, when the remainder of Ψ is evaluated, the strongly peaked portions will not disrupt the numerical processes. We consider here only the distribution function for the penetrating beam. The extension of this treatment to include recoil contributions ought to be straightforward.[5] Our approach to this problem appears somewhat different from that of Manning and Padgett, but conceptually they are the same and our treatment evolved from theirs.

For the sake of convenience, we follow Winterbon, Sigmund, and Sanders (WSS)[6] in presuming that the target material is present on both sides of the source plane. For cases where this is a bad approximation to a beam of particles incident on a target face, the corresponding $\Psi(E,x,\mu)$ will indicate considerable scattering back and forth across the x=o plane.

One way to solve for $\Psi(E,x,\mu)$ is to resolve it into components according to the number of elastic collisions that the beam particles have undergone; that is, we write

$$\Psi = \psi_0 + \psi_1 + \cdots + \psi_{n-1} + \Phi_n \quad . \tag{20}$$

The ψ_0 term represents incident particles that have undergone no elastic collisions, the ψ_s terms, s = 1,2,...,n - 1, represents those that have undergone exactly s elastic collisions, and the Φ_n term represents particles that have undergone n and more collisions. The decision as to how many specific ψ_s terms to evaluate, before attempting to solve for Φ_n, depends on the convenience of calculating the ψ_s quantitites and the degree to which the singular portions of $\Psi(E,x,\mu)$ have been removed.

If we substitute the form (20) into Eq. (18), with the source (19), then the Boltzmann equation can be resolved into a series of successive scattering equations. For convenience, we define the operators

$$\hat{\mathcal{L}}_1 = \mu \frac{\partial}{\partial x} - S(E)\frac{\partial}{\partial E} \tag{21}$$

$$\hat{\mathcal{L}}_2 = N\sigma_T(E) - \frac{dS(E)}{dE} \tag{22}$$

so that Eq. (18) is equivalent to

$$(\hat{\mathcal{L}}_1 + \hat{\mathcal{L}}_2)\ \psi_s(E,x,\mu) = W_{s-1}(E,x,\mu) \quad , \quad s=0,1,\cdots,n-1, \tag{23}$$

$$(\hat{\mathcal{L}}_1 + \hat{\mathcal{L}}_2)\ \Phi_n(E,x,\mu) = W_{n-1}(E,x,\mu) + V_n(E,x,\mu) \tag{24}$$

where

$$W_s(E,x,\mu) = \frac{\mu}{2\pi}\int_E^{\beta E} dE'\ \mathcal{F}(E',E)\int d\hat{v}'\ \mu'^{-1}\ \delta(\hat{v}\cdot\hat{v}' - g(E',E))\ \psi_s(E',x,\mu') \tag{25}$$

$$V_n(E,x,\mu) = \frac{\mu}{2\pi}\int_E^{\beta E} dE'\ \mathcal{F}(E',E)\int d\hat{v}'\ \mu'^{-1}\ \delta(\hat{v}\cdot\hat{v}' - g(E',E))\ \Phi_n(E',x,\mu') \tag{26}$$

and

$$W_{-1}(E,x,\mu) = \mathcal{J}(E,x,\mu). \tag{27}$$

For the case of no elastic collisions, that is, $F(E';E)=0$, all of the terms in Ψ will remain zero, except for the ψ_0 term. The continuous energy loss model for inelastic collisions results in the beam remaining collimated and monochromatic as it penetrates, but with the energy per particle continuously decreasing. If we now imagine that the elastic scattering is turned on, when a particle undergoes its first elastic collision it leaves the ψ_0 term and enters the ψ_1 term. Eventually, after its nth elastic collision, it enters the Φ_n term, which represents it thereafter. Thus, as the beam penetrates deeper into the target, we expect the $\psi_0, \psi_1, \ldots, \psi_{n-1}$ terms to first grow in magnitude and then attenuate, leaving only the Φ_n term deep in the target material.

The approach just described is equivalent to the use of a hierarchy of limiting procedures by Manning and Padgett.

A comment on the handling of the inelastic losses is in order before we proceed to the derivations. The results of the next several sections are obtained for a general inelastic loss law $S(E)$, but, in addition to the general results, we present the specific results for the velocity stopping law

$$S(E) = K E^{\frac{1}{2}}. \tag{28}$$

A velocity stopping law form is given as a primed equation following the general result, wherever appropriate. We do this, firstly, because the velocity stopping law is the form most commonly used to represent inelastic losses at low energies and it is convenient to have the results at hand. Further, the example of this simple form of $S(E)$ serves to elucidate the method we use of solve the resolved Boltzmann equations (Eqs. (23-26)).

IV. THE SOLUTION FOR $\psi_0(E,x,\mu)$

We will solve for $\psi_0(E,x,\mu)$ indeed, for each $\psi_j(E,x,\mu)$ by using the method of characteristics[12-14] of partial differential equation theory. We have adopted this method with little explanation of its use, so the reader may want to examine Refs. (12-14), or others, before proceeding.

The equation satisfied by $\psi_0(E,x,\mu)$ is

$$\mu \frac{\partial}{\partial x}\psi_0(E,x,\mu) - S(E)\frac{\partial}{\partial E}\psi_0 = \Sigma_2\psi_0 + \mathcal{S}(E,x,\mu). \tag{29}$$

The method of characteristics demonstrates that a first order partial differential equation is equivalent to a coupled set of ordinary differential equations; specifically, Eq. (29) is equivalent to

$$\frac{d\mu}{0} = \frac{dx}{\mu} = -\frac{dE}{S(E)} = \frac{d\psi_0}{-\Sigma_2\psi_0 + \mathcal{S}}\ . \tag{30}$$

The first expression merely indicates that we may consider the direction cosine μ as a parameter instead of as a variable. The next pair of equated terms in the string (30) are easily solved, yielding

$$\frac{x}{\mu} - \int_E^{E^*} d\varepsilon\ S^{-1}(\varepsilon) = A = \frac{x}{\mu} - f(E) \tag{31}$$

$$A = \frac{x}{\mu} - \frac{2}{K}\left(E^{*\frac{1}{2}} - E^{\frac{1}{2}}\right) \tag{31'}$$

which defines $f(E)$, where A is an arbitrary constant and E^* is arbitrary except that we take it to be greater than the beam energy E_0. Clearly, $f(E)$ will be a known function, numerically, at least, since $S(E)$ is known.

The method of characteristics has thus indicated that if ψ_0^* is a solution of Eq. (29), then so is $\psi_0^* + \mathcal{f}(A)$, where $\mathcal{f}(A)$ is any arbitrary function of A. That this is true can be seen by substituting an arbitrary function of $A = x/\mu - f(E)$ into Eq. (29), and thus verifying that it is a solution of the homogeneous portion of that equation. This fact allows us to use Eq. (31) to eliminate one of the two variables (x and E) in favor of

the other when we solve for Ψ_0 .

The last equated pair of expressions in Eq. (30) can be written

$$d\Psi_0 = S^{-1}(E)\left[\hat{\mathcal{L}}_2 \Psi_0 - \mathcal{S}\right] dE \, . \tag{32}$$

We introduce the integrating factor $I(E^*,E)$, with

$$I(E^*,E) = \exp\left\{ -\int_E^{E^*} d\varepsilon \, S^{-1}(\varepsilon)\, \hat{\mathcal{L}}_2(\varepsilon) \right\} \tag{33}$$

so that

$$\Psi_0(E,x,\mu) = I(E^*,E)\, \bar{\Psi}_0(E,x,\mu) \tag{34}$$

$$d\bar{\Psi}_0 = -I(E^*,E)\, S^{-1}(E)\, \mathcal{S}(E,x,\mu)\, dE \, . \tag{35}$$

If we insert the explicit form (22) for $\hat{\mathcal{L}}_2$, we see that $I(E^*,E)$ can be written

$$I(E^*,E) = S(E^*)\, R(E^*,E)\, S^{-1}(E) \tag{36}$$

$$R(E^*,E) = \exp\left\{ -\int_E^{E^*} d\varepsilon \, S^{-1}(\varepsilon)\, N\sigma_T(E) \right\} . \tag{37}$$

Upon using expression (19) for $\mathcal{S}$ and using Eq. (31) to eliminate x in favor of E in Eq. (35), we find

$$\bar{\Psi}_0 = B + \int_E^{E^*} d\varepsilon \, I(\varepsilon,E^*)\, S^{-1}(\varepsilon)\, \delta(\mu-1)\, \delta(\varepsilon-E_0)\, \delta(\mu(A+g(\varepsilon))) \tag{38}$$

where B is an arbitrary constant; upon performing the integration we obtain

$$\bar{\Psi}_0 = B + U(E_0 - E)\, I(E_0,E^*)\, S^{-1}(E_0)\, \delta(\mu-1)\, \delta(A+g(E_0)) \, . \tag{39}$$

Our boundary conditions are simply that the only particles of type "2" in the system are those that arise from the source $\mathcal{S}$. Clearly, then, we have that the inhomogeneous contribution vanishes; that is, we have $B=0$. By using expression (31) we have, with $\mu=1$, that

$$A + f(E_0) = x - \int_E^{E_0} d\varepsilon \; S^{-1}(\varepsilon) \tag{40}$$

$$A + f(E_0) = x - 2(E_0^{\frac{1}{2}} - E^{\frac{1}{2}})/K \, . \tag{40'}$$

Let us define $E_1(x)$ to be a function that, when substituted for E in Eq. (40), makes the expression vanish. Thus we can write, for $E \approx E_1(x)$,

$$x - \int_E^{E_0} d\varepsilon \; S^{-1}(\varepsilon) \approx (E - E_1(x)) \, S^{-1}(E_1(x)) \, . \tag{41}$$

(For the velocity stopping law, we have

$$E_1(x) = (E_0^{\frac{1}{2}} - \tfrac{1}{2} K x)^2 \tag{41'}$$

as the explicit form of $E_1(x)$.)

Upon combining these several results, we obtain

$$\psi_0(E,x,\mu) = \delta(\mu - 1) \, U(x) \, \delta(E - E_1(x)) \, R(E_0, E) \, . \tag{42}$$

(We note that $U(E_0 - E_1(x)) = U(x)$.) We see that each beam ion, prior to an elastic collision, traverses the target material with its direction of motion unaltered but with its energy diminished by electronic losses according to the prescription $E = E_1(x)$. Elastic collisions lead to the attentuation of the ψ_0 component of the flux by the factor $R(E_0, E)$.

Finally, we note that we can set $E' = E_0$ with no loss of generality.

V. THE SOLUTION FOR $\psi_1(E,x,\mu)$

If we substitute the result (42) into Eq. (25), we obtain

$$W_0(E,x,\mu) = \mu \, \delta(\mu - g(E_1(x), E)) \, U(x) \, R(E_0, E_1(x)) \, \mathcal{F}(E_1(x), E) \, . \tag{43}$$

We can now solve Eq. (23) for ψ_1 by using the method of characteristics. The procedure is virtually identical to that used for the ψ_0 case, so that

we obtain

$$\Psi_1(E,x,\mu) = S^{-1}(E)\int_E^{E_0} d\varepsilon \;\; P(\varepsilon,E)\; W_0(\varepsilon, X(\varepsilon), \mu) \tag{44}$$

where

$$X(\varepsilon) = x - \mu\left(f(E) - f(\varepsilon)\right) \tag{45}$$

$$X(\varepsilon) = x - \mu\left(\varepsilon^{1/2} - E^{1/2}\right)/K \; . \tag{45'}$$

The function $\varepsilon_1 = \varepsilon_1(X(\varepsilon))$, which replaces $E_1(x)$ in W_0 in the integrand of Eq. (44), is determined by

$$X(\varepsilon) = f(\varepsilon_1) \tag{46}$$

$$\varepsilon_1 = \left[\left(E_1(x)\right)^{1/2} + \mu\left(\varepsilon^{1/2} - E^{1/2}\right)\right]^2 \tag{46'}$$

where x, μ, ε and E are given.

The integrand in Eq. (44) contains the factor $\delta(\mu - g(\varepsilon_1, \varepsilon))$. By using the expression (11) for , and defining

$$h = (\varepsilon/\varepsilon_1)^{1/2} \; , \tag{47}$$

we find that the values of h that satisfy the delta function are

$$\bar{h} = h_\pm = \left(\mu \pm (\mu^2 + M^2 - 1)^{1/2}\right)/(M+1) \; . \tag{48}$$

The appropriate sign to be used in Eq. (48) for h is indicated in Table 1; note that μ is double valued as a function of h for the case $M<1$. The quantity h is either positive or zero, and is only zero for the case of 90° scattering with $M=1$. The value $\bar{\varepsilon}_1$ of ε_1 corresponding to $h = \bar{h}$ is obtained from Eqs. (47,48); that is,

$$f(\bar{\varepsilon}_1) = x - \mu\left(f(E) - f(\bar{h}^2 \bar{\varepsilon}_1)\right) \tag{49}$$

$$\bar{\varepsilon}_1 = \left[\left(E_1(x)^{1/2} - \mu E^{1/2}\right)/(1 - \mu h)\right]^2 . \tag{49'}$$

Table 1

Dependence of h on μ and M

M	θ	μ	h
>1	$\pi \ge \theta \ge 0$	$-1 \le \mu \le 1$	$\beta^{-\frac{1}{2}} \le h = h_+ \le 1$
$=1$	$\frac{\pi}{2} \ge \theta \ge 0$	$0 \le \mu \le 1$	$0 \le h = \mu \le 1$
<1	$0 \le \theta \le \theta_m$	$1 \ge \mu \ge (1-M^2)^{\frac{1}{2}}$	$\beta^{-\frac{1}{2}} \le h = h_- \le \beta^{-\frac{1}{4}}$
	$\theta_m \ge \theta \ge 0$	$(1-M^2)^{\frac{1}{2}} \le \mu \le 1$	$\beta^{-\frac{1}{4}} \le h = h_+ \le 1$

$$\left(\theta_m = \cos^{-1}(1-M^2)^{\frac{1}{2}} \right) \qquad \left(h_\pm = (M+1)^{-1}\left[\mu \pm (\mu^2+M^2-1)^{\frac{1}{2}}\right] \right)$$

We can now write

$$\delta(\mu - g(\varepsilon_1, \varepsilon)) = P(E,x,\mu)\ \delta(\varepsilon - \bar{\varepsilon}) \tag{50}$$

$$P(E,x,\mu) = \frac{4\bar{\varepsilon}\bar{h}}{M+1}\left|\left(1-\mu\bar{h}^2 S^{-1}(\bar{\varepsilon}) S(\bar{\varepsilon}_1)\right)\left(\bar{h}^2 + \frac{M-1}{M+1}\right)\right|^{-1}, \tag{51}$$

where

$$\bar{\varepsilon} = \bar{h}^2\ \bar{\varepsilon}_1 . \tag{52}$$

By combining these results we obtain

$$\Psi_1(E,x,\mu) = \mu\ S^{-1}(E)\ U(\beta\bar{\varepsilon} - \bar{\varepsilon}_1)\ U(E_0 - \bar{\varepsilon}_1)\ U(\bar{\varepsilon}_1)\ U(\mu^{-1}(x-\bar{x})) \tag{53}$$

$$\times\ R(E_0, \bar{\varepsilon}_1)\quad \mathcal{F}(\bar{\varepsilon}_1, \bar{\varepsilon})\quad R(\bar{\varepsilon}, E)\quad P(E,x,\mu)$$

where $\bar{\varepsilon}_1$ and $\bar{\varepsilon}$ are given by Eqs. (49,52) and where

$$\bar{x} = x - \mu\,(g(E) - g(\bar{\varepsilon})) \tag{54}$$

$$\bar{x} = x - \mu\,(\bar{\varepsilon}^{\frac{1}{2}} - E^{\frac{1}{2}})/K \,. \tag{54'}$$

The physical interpretation of the expression for $\psi_1(E,x,\mu)$ is straightforward. Suppose we ask what the once scattered flux is at depth x with energy E and direction cosine μ. Given a particular form for $S(E)$, there is, at most, one way that a beam particle can scatter just once and have the coordinates (E,x,μ). Specifically, it travels without scattering from $(E_0,0,1)$ to $(\bar{\varepsilon}_1,\bar{x},1)$ and there scatters to $(\bar{\varepsilon},\bar{x},\mu)$, after which it travels without further elastic collisions to (E,x,μ). The step function $U(\mu^{-1}(x-\bar{x}))$, which arises from Eq. (54), reflects the fact that $\bar{\varepsilon}$ must be greater than or equal to E. The step function $U(\bar{\varepsilon}_1)$, which arises from Eq. (49), merely indicates that the beam particle must not have come to rest before it scattered. The explicit presence of these step functions is useful when evaluating integrals over $\psi_1(E,x,\mu)$.

VI. THE SOLUTIONS FOR $\psi_2,\ldots,\psi_{n-1},\Psi_n$

The formal solutions for $\psi_s,\ s=2,\ldots,n-1$ are the same as the first steps in the solution for ψ_1. The method of characteristics yields

$$\psi_s(E,x,\mu) = S^{-1}(E)\int_E^{\beta E} d\varepsilon\ R(\varepsilon,E)\,W_{s-1}(\varepsilon, X(\varepsilon), \mu) \tag{55}$$

where $X(\varepsilon)$ is again given by Eq. (45). For these cases the W_{s-1} functions contain no delta functions, as W_{-1} and W_0 did, so that each must be evaluated numerically.

Similarly, the expression for $\Psi_n(E,x,\mu)$ is

$$\Psi_n(E,x,\mu) = S^{-1}(E)\int_E^{\beta E} d\varepsilon\ R(\varepsilon,E)\left[W_{n-1}(\varepsilon,X(\varepsilon),\mu) + V_n(\varepsilon,X(\varepsilon),\mu)\right], \tag{56}$$

which is an integral equation for Ψ_n.

Generally, one would not continue the iteration process to large n in order to solve for Ψ deep in the target; too much computer time would be

needed to calculate the Ψ_2 quantities. The main purpose of the expansion is to evaluate the first few terms, so that the remaining portion of the distribution function, which is found be solving an integral equation, no longer possesses the singular behavior of the first few terms.

VII. SAMPLE CALCULATIONS

We have evaluated the Ψ_0 and Ψ_1 contributions to Ψ for a number of values of the beam energy and of the mass ratio. We will present the results for one case in some detail and then take note of the differences that arise when M and E_0 are varied. The purpose of these calculations is to illustrate the sharply peaked behavior of Ψ near the target surface.

For the elastic cross section we use the form due to Lindhard, Nielsen and Scharff (LNS),[15] which is discussed in Appendix B. For the inelastic losses we use the velocity stopping law of Eq. (28). The constant K in this equation depends on the charges and masses of the interacting ions. The LSS expression for K, as well as their criterion for the applicability of this law, are also given in Apprendix B. The relations between $\bar{\epsilon}_1$, $\bar{\epsilon}$, and $\bar{x}$ and E, x, and μ can be found in Eqs. (48, 49', 52, 54') with $E_1(x)$ given by

$$E_1(x) = \left(E_0^{\frac{1}{2}} - \tfrac{1}{2}Kx\right)^2 . \tag{57}$$

Unless otherwise noted, all energies are in units of MeV and all depths in microns.

We consider the case of 100 keV helium ions incident on a pure nickel target. We take the energy transfer cutoff T_1, which is discussed in Appendix B, to be 25 ev.

Figure 1a shows the region of the E-θ plane for which $\Psi_1(E,x,\mu)$ is non-zero; the restrictions that form the boundaries in the figure are also shown. These boundaries arise from the step functions that appear in Eq. (53). The plot shown is for a depth of 0.04 microns (E_1= 87.998 keV), but the results at other depths are similar. Figure 1b is a magnified view of the small angle portion of Fig. 1a. We see that the T_1 cutoff allows a minimum scattering angle of θ_{min} = 3.47^0. More generally, this minimum angle is given by

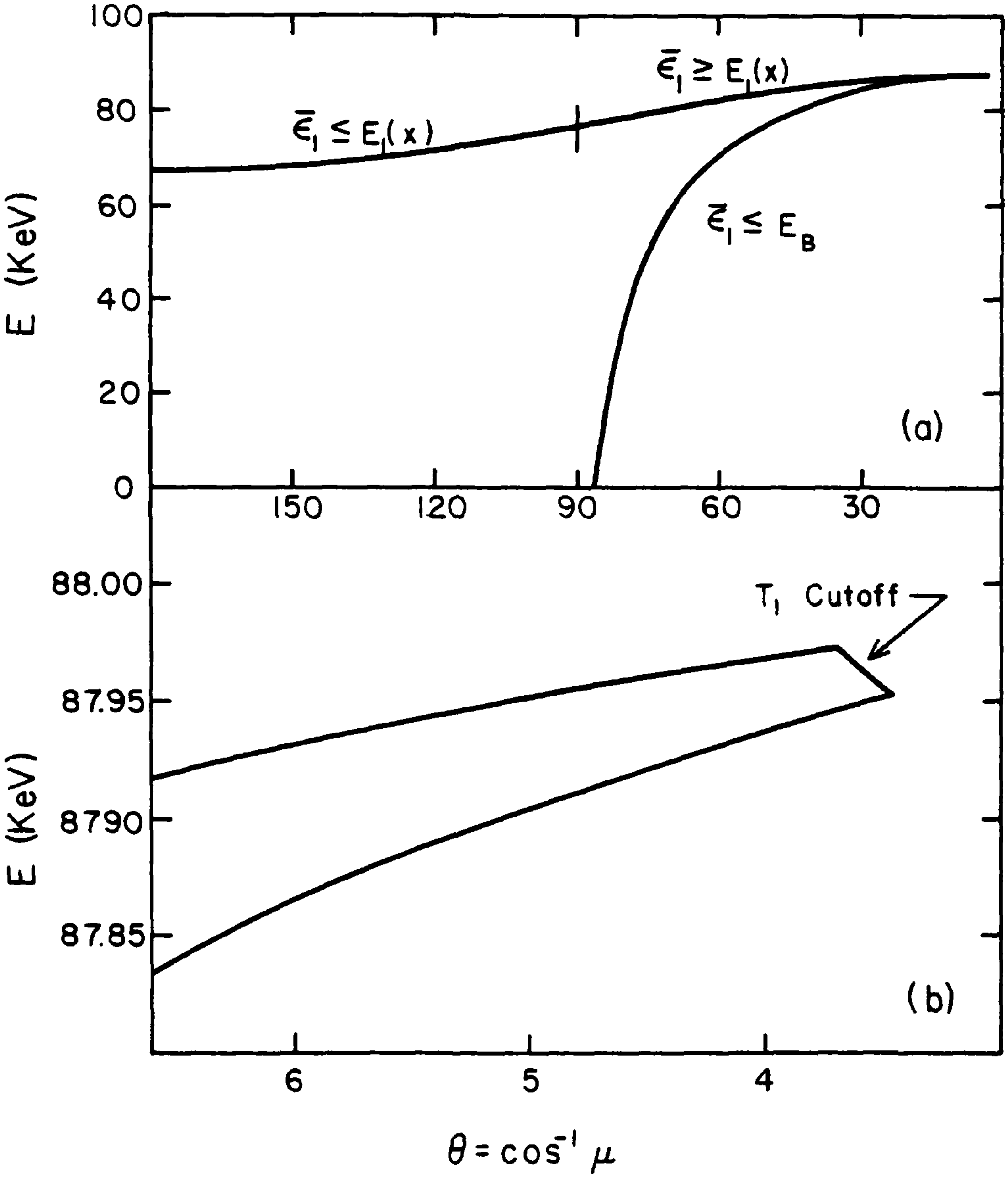

Fig. 1. (a) Region of the E-θ plane for which $\psi_1(E,x,\mu)$ is non-zero for 100 keV He incident on Ni at x = .04. (b) Expanded view of the small angle portion of (a).

$$\theta_{min} = \cos^{-1}[\tfrac{1}{2}(M+1)(1-T_1/E_1) - \tfrac{1}{2}(M-1)(1-T_1/E_1)^{-1}]. \qquad (58)$$

We next present a plot of the logarithm of the absolute value of the quantity

$$J_1(x,\mu) = \int_0^{E_B} dE \ \psi_1(E,x,\mu) \qquad (59)$$

which measures the particle flux of all energies at the depth x and in the direction $\theta=\cos^{-1}\mu$. Figure 2 shows that almost all of the ψ_1 flux is concentrated at very small angles and, consequently, the flux is concentrated in a very narrow energy range. In Fig. 3, we show an isometric plot of the logarithm of $\psi_1(E,x,\mu)$ for $0° \leq \theta \leq 90°$ at x = 0.04 microns. We again see the strong peaking for small scattering angle. In the region where E can approach zero ($\theta \geq 86.2°$), ψ_1 blows up as the minus one half power of E, which is depicted by the arrow rising from this region in Fig. 3. The constant of proportionality is so small, however, that we can infer that only a negligible faction of the total flux comes to rest at this depth.

We have made similar calculations of ψ_1 for a variety of values of the mass ratio and of the beam energy E_B. The results are as expected. As the beam energy increases, the peaking also increases, due in part to the decrease in the minimum scattering angle. As the incident particle becomes more massive, in comparison to the target particles, the flux again is more strongly peaked in the forward direction. This is due both to the reduction in the allowed minimum scattering angle and to the fact that the kinematics favor smaller angle scattering as M decreases.

In general, the single elastic scattering contributions to $\psi_1(E,x,\mu)$ is sharply peaked in the forward direction, with most of the flux concentrated at angles near the minimum scattering angle. This angle is determined by the cutoff, which precludes elastic collisions in which the primary knock-on atoms would have less energy than is necessary to allow them to escape from their lattice sites.

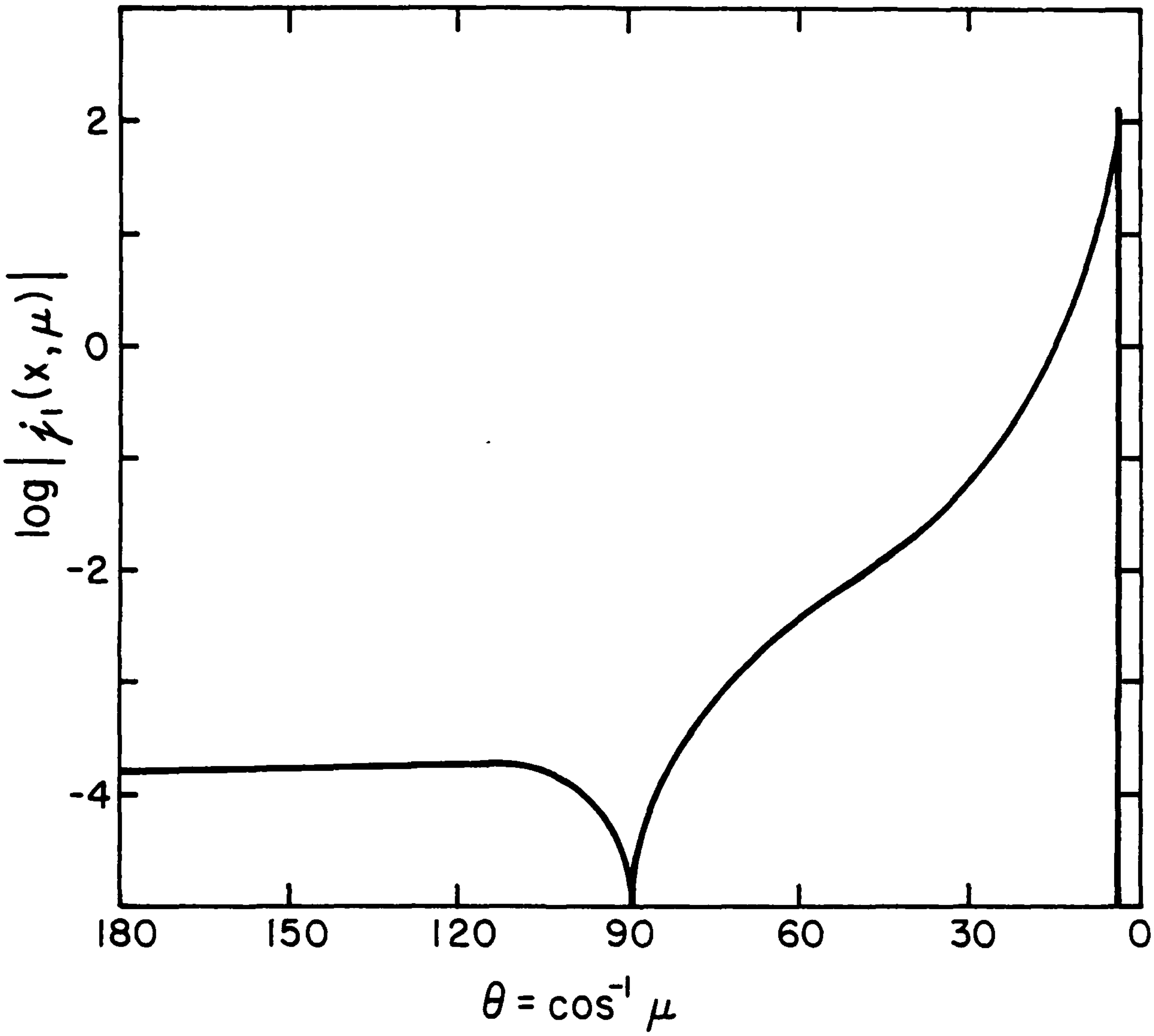

Fig. 2. Plot of log $|j_1(x,\mu)|$ vs. angle for 100 KeV He incident on Ni at x=0.04.

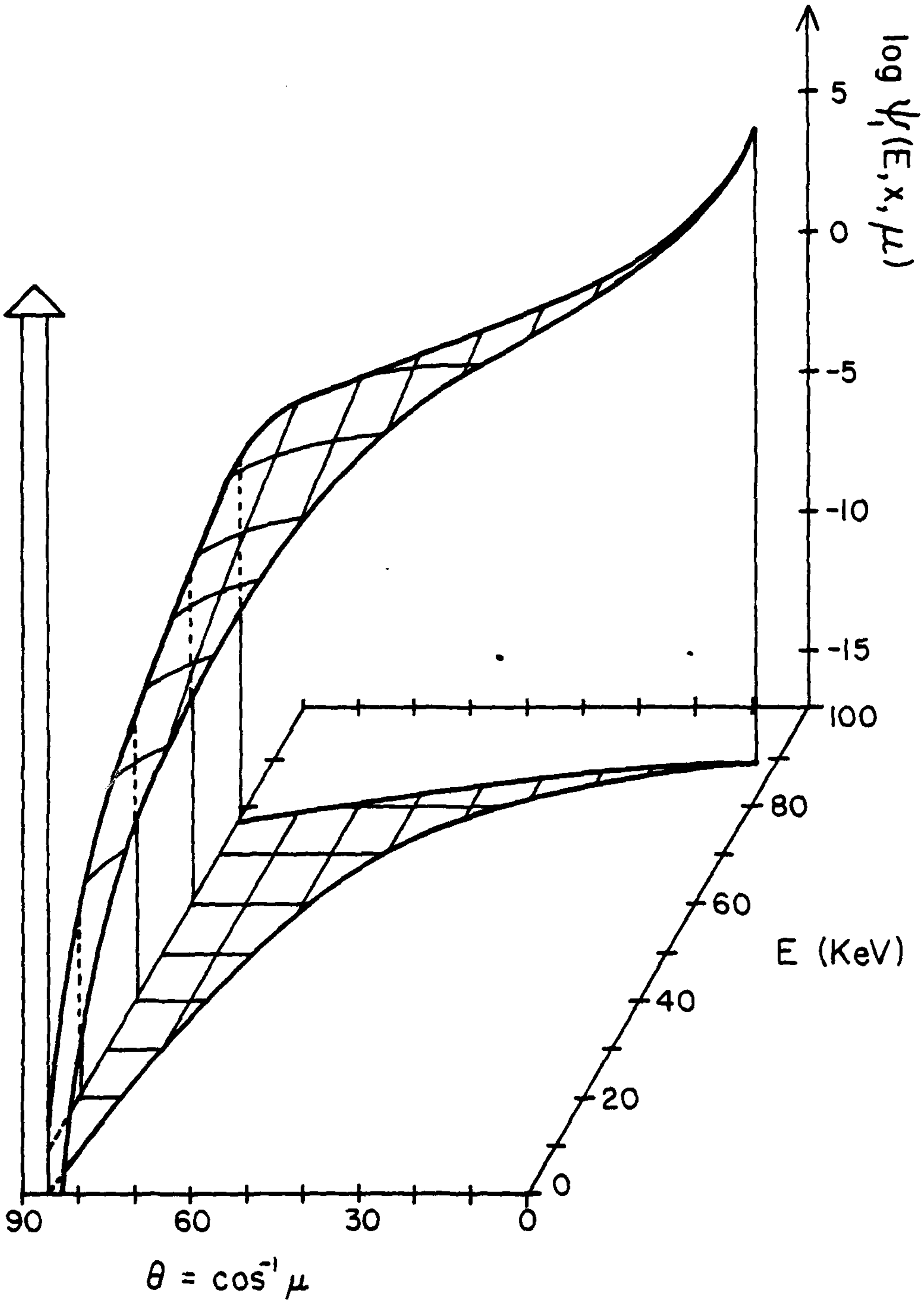

Fig. 3 Plot of log $\psi_1(E,x,\mu)$ vs. angle for 100 keV He incident on Ni at x=0.04.

VIII. CONCLUSIONS

The present work can serve as the starting point for a number of investigations. One could solve for $\Psi(E,x,\mu)$ by iteration, that is, by calculating successive ψ_s terms. Near the surface, only a few iterations would be needed, so that, for instance, one could obtain a reliable estimate of the distribution of beam ions that are scattered out of the target. Some account of true surface effects would be needed. It would also be straightforward[5] to include the distribution function for the target atoms. This distribution would have a term, analogous to our term, that described exactly the distribution of target atoms that had been struck by beam ions, but had suffered no further elastic collisions with other target atoms. Successive contributions to the target atom flux could be found by iteraction. Near the surface, this calculation would yield the distribution of sputtered atoms. In principle, one could solve for Ψ at all depths by iteration, but the cost in computer time and the danger of accumulating errors makes this approach unworthy of the effort.

The more common approach would be to expand Φ_n in series of orthogonal polynomials; Legendre polynomials in μ and Hermite polynomials in x, for example. This method would replace the integral equation (56) with a coupled set of much simpler integral equations for the coefficients of the expansion. Another, related, approach may prove valuable. We noted in the last section that the ψ_1 contribution to the flux is strongly peaked in the forward direction. Clearly, the Φ_n contribution will also be peaked in the forward direction for energies near the beam energy. Given this situation, it may be useful to expand $\Phi_n(E,x,\mu)$ as a function of μ in a series of Jacobi polynomials. These polynomials, which are a generalization of the Legendre polynomials, have the property that an inherent peaking can be built into them.[16] By incorporating the peaking behavior directly into the expansion functions, we would hope to reduce considerably the number of terms necessary to represent the distribution function accurately.

ACKNOWLEDGMENTS

I would like to thank Irwin Manning for suggesting this problem and him and D.W. Padgett for many discussions concerning their method of approaching the solution of the Boltzmann equation representing heavy ion penetration of an amorphous target.

APPENDIX A. CONTINUOUS ENERGY LOSS MODEL FOR INELASTIC COLLISIONS

From Eq. (7) and the discussion following it we see that the inelastic (electronic) cross section furnishes two contributions to the Boltzmann equation; one arises from the total cross section term on the left-hand side of the Boltzmann equation and the other from the scattering term on the right-hand side. We write these as

$$C_L = N \sigma_{s,in}(E) \Psi(E,x,\mu) \tag{A1}$$

$$C_R = N \mu v \int d^3v' \; \sigma_{in}(\underline{v}' \to \underline{v}) \; (\mu' v')^{-1} \; \Psi(E',x,\mu') \tag{A2}$$

where

$$\sigma_{s,in}(E') = \int d^3v \;\; \sigma_{in}(\underline{v}' \to \underline{v}) . \tag{A3}$$

As indicated in Eq. (10), we wish the inelastic cross section to satisfy

$$S(E') = N \int d^3v \;\; (E' - E) \; \sigma_{in}(\underline{v}' \to \underline{v}) \tag{A4}$$

where $S(E)$ is the rate of energy loss of beam ions to purely inelastic collisions.[10]

Following Symon[11] we use a continuous energy loss model. A general form for $\sigma_{in}(\underline{v}' \to \underline{v})$ which can be made to satisfy Eqs. (A3,A4) is

$$\sigma_{in}(\underline{v}' \to \underline{v}) = \sigma_{s,in}(E') \, \delta(\Omega_v - \Omega_{v'}) \left[f_2(E') \, \delta(v - v') + f_1(E') \frac{d}{dv} \delta(v - v') \right] \tag{A5}$$

where f_1 and f_2 are yet to be determined. Upon substituting the form (A5) into Eq. (A3) we find

$$1 = \int_0^\infty dv \; v^2 \; \left[f_2(E') \, \delta(v - v') \; + f_1(E') \frac{d}{dv} \delta(v - v') \right] . \tag{A6}$$

We can evaluate the integral in Eq. (A6) by using the relations

$$\int_{-\infty}^{\infty} dx \;\; g(x) \;\; \delta(x - y) \;\; = \; g(y) \tag{A7}$$

$$\int_{-\infty}^{\infty} dx\, g(x) \frac{d}{dx} \delta(x-y) = -\int_{-\infty}^{\infty} dx\, \delta(x-y)\, g'(x) = -g'(y) \tag{A8}$$

so that we obtain

$$I = v'^2 f_2(E') - 2v' f_1(E'). \tag{A9}$$

Thus $f_2(E)$ is determined as a functional of $f_1(E)$, which is still undetermined.

After substituting the form (A5) into Eq. (A4), we obtain

$$S(E') = N m_1 v'^3 \sigma_{S,in}(E') f_1(E'). \tag{A10}$$

In similar fashion we can evaluate C_R, obtaining

$$\begin{aligned} C_R = N\Big[& v \frac{\partial}{\partial v} \Big(v\, \sigma_{S,in}(E) f_1(E)\, \Psi(E,x,\mu) \Big) \\ & + v^2 \sigma_{S,in}(E) f_2(E)\, \Psi(E,x,\mu) \Big] \end{aligned} \tag{A11}$$

which becomes, upon inverting the result (A9),

$$\begin{aligned} C_R = {} & 3Nv\, \sigma_{S,in}(E) f_1(E)\, \Psi(E,x,\mu) \\ & + Nv^2 \frac{\partial}{\partial v} \Big(\sigma_{S,in}(E) f_1(E)\, \Psi(E,x,\mu) \Big) + N \sigma_{S,in}(E)\, \Psi(E,x,\mu). \end{aligned} \tag{A12}$$

By combining Eq. (A10) with Eq. (A12) we find that

$$C_R = N \sigma_{S,in}(E)\, \Psi(E,x,\mu) + \frac{\partial}{\partial E} \Big(S(E)\, \Psi(E,x,\mu) \Big). \tag{A13}$$

We see that when C_L and C_R are substituted into the Boltzmann equation, the first term in C_R cancels C_L, so that the final form for Boltzmann equation is that given in Eq. (11).

We note that $\sigma_{S,in}$, which in the case of elastic scattering would correspond to the total cross section, is an arbitrary quantity, depending on the choice of the function $f_1(E)$. We conclude that the concept of a

total cross section has no meaning for a differential cross section of the form (A5).

APPENDIX B. LINDHARD CROSS SECTION

The Lindhard, Nielsen, and Scharff (LNS)[15] differential cross section for elastic atomic scattering is given by

$$d\sigma_{LNS}(\underline{v}' \to \underline{v}) = \tfrac{1}{2}\pi a^2 t^{-3/2} f(t^{1/2}) \left| dt/dv \right| (2\pi)^{-1} \delta(\hat{\underline{v}} \cdot \hat{v}' - g(E';E))\, dv\, d\hat{v} \tag{B1}$$

where

$$t = E'(E'-E)/(\gamma E_L^2) . \tag{B2}$$

The Lindhard unit of energy is given by

$$E_L = Z_1 Z_2 \, (e^2/a) \, (m_1 + m_2)/m_2 \tag{B3}$$

$$a = 0.8853 \, a_0 \, Z^{-\frac{1}{3}} \tag{B4}$$

$$Z = (Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}})^{\frac{3}{2}} \tag{B5}$$

$$\gamma = 4 m_1 m_2 \, (m_1 + m_2)^{-2} \tag{B6}$$

where a_0 is the Bohr radius for the hydrogen atom. The function $f(t^{\frac{1}{2}})$ is obtained by LNS from a Thomas-Fermi model of atomic scattering and is supplied by them in tabular form.

When the collision kernal $F(E';E)$ is expressed in terms of the LNS cross section we obtain

$$F(E';E) = \tfrac{1}{2} \pi a^2 v^{-2} t^{-\frac{3}{2}} f(t^{\frac{1}{2}}) \left| dt/dv \right| \tag{B7}$$

so that

$$d\sigma_{LNS}(\underline{v}' \to \underline{v}) = (2\pi)^{-1} \delta(\hat{v} \cdot \hat{v}' - g(E';E)) \; F(E';E) \, d^3v . \tag{B8}$$

The total cross section is given by

$$\sigma_T(E') = \pi a^2 \int_{\eta_1}^{\eta_2} d\eta \ \eta^{-2} \ f(\eta) \tag{B9}$$

where

$$\eta_1 = (E' T_1 / (\gamma E_L^2))^{\frac{1}{2}} \ , \quad \eta_2 = E'/E_L \ . \tag{B10}$$

Since the LNS cross section blows up as the energy transfer $T = E'-E$ goes to zero, it is necessary to introduce a minimum energy transfer T_1. The imposition of the cutoff T_1 is less arbitrary then it might seem since T_1 can be related to the displacement energy E_d, which is the average energy needed to displace a target atom from its lattice site.

The function $f(t^{\frac{1}{2}})$ is presented in tabular form by LNS, but it is more convenient to use the analytical fit to $f(t^{\frac{1}{2}})$ provided by Winterbon, Sigmund, and Sanders (WSS).[6] Specifically, they give

$$f(t^{\frac{1}{2}}) = \lambda t^{\frac{1}{6}} \left[1 + (2\lambda t^{\frac{2}{3}})^{\frac{2}{3}} \right]^{-3/2} \tag{B11}$$

with $\lambda = 1.309$. An explicit expression for the total cross section corresponding to the WSS choice for $f(t^{\frac{1}{2}})$ has been developed.[17]

LSS[10] provide an expression for the constant that appears in the velocity stopping law. If we write

$$S(E) = K \ E^{\frac{1}{2}} \tag{B12}$$

with $S(E)$ in units of MeV per micron and E in MeV, we have

$$K = 1.216 \cdot 10^{-23} \ Z_1^{\frac{1}{6}} \ (Z_1 Z_2 / Z) N(cm^{-3}) \ (m_1(amu))^{-\frac{1}{2}} . \tag{B13}$$

LSS give

$$E < 0.025 \ Z_1^{\frac{4}{3}} \ m_1 \ (amu) \tag{B14}$$

as a rough criterion for the applicability of the stopping law (B12).

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